

CLAIMS

What is claimed is:

1. A method for accounting for adducts in spectra to make library searching more reliable, said method including the steps of:

(i) collecting multiple spectra at varying collision energies from a mass spectrometer;

(ii) identifying the pseudo molecular ion;

(iii) using said multiple spectra to create reduced spectra;

(iv) creating a composite spectrum out of said reduced spectra;

(v) searching against a library of known composite spectra for said composite spectrum; and

(vi) assigning a match quality value, said match quality value indicative of a measure of the fit between the composite spectrum and the library of known composite spectra.

2. The method according to claim 1, wherein the pseudo molecular ion is identified in the multiple spectra with the lowest collision energy for which one or more ions are produced.

3. The method according to claim 1, wherein said reduced spectra ignore ions with masses above the pseudo molecular ion.

4. The method according to claim 1, wherein said pseudo molecular ion is a pseudo molecular ion cluster, said molecular ion cluster comprising a most abundant molecular ion and all related ions resulting from the inclusion of naturally occurring isotopes of elements that make up said most abundant molecular ion.

5. The method according to claim 1, wherein the steps are performed by an executable program.

6. The method according to claim 1, wherein the step of assigning a match quality value further includes the factoring in the presence of adduct, dimer, or oligomer ions in the original spectra into the match quality value, wherein said presence of adduct, dimer, or oligomer ions is assigned a weighting factor of small significance.

7. The method according to claim 1, wherein said mass spectrometer is a liquid chromatograph-mass spectrometer.

8. The method according to claim 1, wherein said multiple spectra are generated from atmospheric pressure ionization and collision induced dissociation.

9. A method for identifying a pseudo molecular ion in a spectrum, said method including the steps of:

(i) creating a composite spectrum from multiple spectra, said multiple spectra collected at varying collision energies from a mass spectrometer; and

(ii) using a first dynamic algorithm for assigning a degree of importance to ions depending upon the identity of said ions.

10. The method according to claim 9, further including the step of:

(iii) using a second dynamic algorithm for assigning a degree of importance to the ion ratios depending upon the identity of said ions.

11. The method according to claim 10, further including the step of:

(iv) searching said composite spectrum against a library of composite spectra, said library of composite spectra including adduct, dimer, and oligomer ions.

12. The method according to claim 11, further including the step of:

(vi) determining a match quality value, said match quality value taking into account any or all ions in the spectrum along with the ions' ratios and degrees of importance.

13. The method according to claim 10 wherein the ratios of adduct, dimer, and/or oligomer ions to each other or to the pseudo molecular ion are given a weighting factor of small significance.

14. The method according to claim 10 wherein the ion ratios for the pseudo molecular ion and fragment ions are given a weighting factor of large significance.

15. The method according to claim 9, wherein said mass spectrometer is a liquid chromatograph-mass spectrometer.

16. The method according to claim 9, wherein said multiple spectra are generated from atmospheric pressure ionization and collision induced dissociation.

17. The method according to claim 9, wherein the steps are performed by an executable program.

18. The method according to claim 12, wherein said first dynamic algorithm and said second dynamic algorithm are modified and said step of determining a match quality value is repeated.

19. A system for searching a reference library of known compounds, said system including:

(i) a mass spectrometer, said mass spectrometer generating a composite spectrum for an unknown compound, said composite spectrum including a pseudo molecular ion and fragment ions;

(ii) a reference library; and

(iii) a computer,

(a) for assigning a degree of importance to the ion ratios depending upon the identity of said ions, and

(b) searching said reference library using said composite spectra from said mass spectrometer.

20. The system according to claim 19, wherein said computer determines a match quality value, said match quality value taking into account any or all ions in the composite spectrum along with the ions' ratios.

21. The system according to claim 19, wherein said reference library stores multiple spectra for each known compound.

22. The system according to claim 19, wherein said mass spectrometer is a liquid chromatograph-mass spectrometer.

23. The system according to claim 19, wherein said composite spectra are generated from atmospheric pressure ionization and collision induced dissociation.

24. The system according to claim 20, wherein the ratios of adduct, dimer, and/or oligomer ions to each other or to the pseudo molecular ion are given a weighting factor of small significance in the determination of said match quality value.

25. The system according to claim 20, wherein the ion ratios for the pseudo molecular ion and fragment ions are given a weighting factor of large significance in the determination of said match quality value.

26. A computer readable medium, said computer readable medium including instructions to cause a computer to:

(i) create a composite spectrum from multiple spectra, said multiple spectra collected at varying collision energies; and

(ii) use first a dynamic algorithm for assigning a degree of importance to ions depending upon the identity of said ions.

27. The computer readable medium according to claim 26, further including instructions to cause said computer to:

(iii) use a second dynamic algorithm for assigning a degree of importance to the ion ratios depending upon the identity of said ions.

28. The computer readable medium according to claim 27, further including instructions to cause said computer to:

(iv) search said composite spectrum against a library of composite spectra, said library of composite spectra including adduct, dimer, and oligomer ions.

29. The computer readable medium according to claim 28, further including instructions to cause said computer to:

(v) determine a match quality value, said match quality value taking into account any or all ions in the spectrum along with the ions' ratios.

30. The computer readable medium according to claim 29, wherein the ratios of adduct, dimer, and/or oligomer ions to each other or to the pseudo molecular ion are given a weighting factor of small significance in the determination of said match quality value.

31. The computer readable medium according to claim 29, wherein the ion ratios for the pseudo molecular ion and fragment ions are given a weighting factor of large significance in the determination of said match quality value.